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14. ABSTRACT

In an attempt to develop a viable option for complex turbulent combustion research, the flamelet concept is investigated by developing an interdisciplinary modeling and simulation capability via local grid refinement technique. The inherent deficiency at the grid block interface of the local polynomial refinement approach using the Gauss Quadrature formulation is remedied by a differential reconstruction scheme. The symmetry, coercivity, boundness, and adjoint consistency conditions of solutions at the grid block interface for combustion simulation are enforced for the diffusion dominant equation. A multiple-point, unequal spaced, differencing reconstruction approximation to preserve the spectral accurate and to increase computationally efficient is achieved and systematically validated by the L2 norm projection approach. The developed numerical scheme has been demonstrated to retain comparable spectral accuracy and is thrice more computationally efficient than the classic approach. The intrinsic behavior of the unique algorithm has successfully applied to the counter-flow, air-hydrogen combustion. The highly stretched flame that approaching the extinct limit is successfully simulated; the thin frame structure is captured by the developed numerical method with a greater clarity in resolving the detailed thermal layer of the flame front in a direct comparison with a benchmark of AFRL. The newly developed computational interdisciplinary simulation capability has been transferred to AFRL and applied to a path-finding application for combustion with radiative exchange in hypersonic scramjet.

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Cyber-Based Turbulent Hydrogen Combustion Simulation

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Abstract

The side-by-side computational and experimental combustion research has made remarkable progress in unifying concepts of theoretical foundation for canonical laminar flame phenomena. It is logical to adopt the same approach to turbulent combustion by explore this cutting edge technology [1-3]. However the turbulent structure in combustion presents a formidable challenge. Turbulence is the most complex fluid physics phenomenon of nonlinear dynamics associated with multi-scales in time and space. The drastic difference in flow-field structures between the laminar and turbulent counter-flowing fuel injection is clearly illustrated in figure 1. As a consequence, it has long been recognized as the pacing item in computational fluid dynamics (CFD) [1]. This urgent scientific need for technologic advancement is far from being met. Two fundamental approaches have been developed: the Direct Numerical Simulation (DNS) [4,5] and the Large Eddy Simulation (LES) techniques [6,7]. According to the Kolmogorov micro-scales formulation, the ratio of the extreme length scales is proportional to three-quarter power of the characteristic Reynolds number, $Re^{3/4}$ of a turbulent flowfield. To resolve all scales for three-dimensional motion, the number of grid points required becomes astronomical to be a practical modeling and simulation tool [1,4]. In principle, LES can accurately compute the contribution of the large energy-carrying structures for momentum and energy transfer if numerical error is minimized. Meanwhile, the fine-scale structures of combustion depend upon intermolecular interactions such as transport properties and chemical reaction beneath the molecular scales, which must be modeled [2-11]. Thus, the required computational resource is also prohibitive for practical application at the present time.

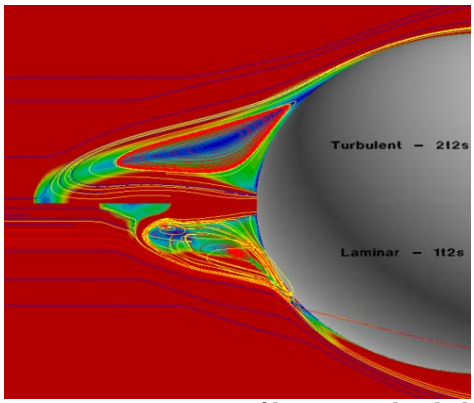

Figure 1. Comparison of laminar and turbulent Counter-flowing injection

An alternative description for turbulent flames is the concept of laminar flamelet, which has been introduced by Peters [2] as an asymptotic concept. This idea is built on the premises that combustion takes place within asymptotically thin layers embedded in the turbulent flow. Therefore the local instantaneous composition of reactants and temperatures of the non-premixed process could be identically modeled as that in a stretched laminar flame. A necessary condition for the flamelet concept to be validated is that the characteristic dimension of the reaction zone must be thinner than the Kolmogorov length scale.

However, Bilger has shown the reaction zone of the flamelet is not necessary asymptotically thin due the reverse reactions [3]. It is known from numerous calculations; the minimum reaction zone for hydrogen flames has a thickness from 0.5 to 1.0 mm that is aerodynamically stretched [8-10]. Recent numerical simulations of

vortex-flame interaction by Katta el al [8] indicate that when the vortices are smaller than millimeter in dimension will not stretch a laminar non-premixed flame but destroy the flame structure in the process. This finding is very interesting it also raises the question whether the laminar-flamelet theory is applicable to turbulent combustion [9]. In order to further substantiate the discovery, a local highly refined grid spacing algorithm of a spectral-like numerical resolution together with a refined diffusion model becomes necessary [8-10]. Since the chemical reaction occurs beneath the molecular scales which is irresolvable by the classic theory of gas kinetics and must be augmented by models of chemical kinetics. Fortunately, this scientific disciplinary has been developed by combustion communities, the reaction rate of the chemical kinetics and the molecular and atomic diffusion model can be accessed through the Cyber space [11,12]. The present research is therefore required only to focus on the development of a high resolution algorithm that is supported by extremely fine local mesh spacing for combustion simulation.

The formulation of Gauss quadrature is known for its high numerical resolution in performing integration between intervals of a real function. The analytic formation is expressed by the Newton's division-difference form on unequal roots of the adopted orthogonal polynomial [13,14]. The basic formulation however is applicable to derivative calculations for any function within the locally refined domain [15-19]. The calculated derivative by this approach can yield a spectral-like resolution more accurate than most high-order numerical schemes and the accuracy is controlled solely by the degrees of the adopted polynomial. For this reason, the ability to refine local grid spacing within an investigated domain using an orthogonal polynomial is also unsuppressed [18,19]. In general, the solutions between immediately adjacent domains are discontinuous. In applying this approach to solve hyperbolic partial differential equations, the conservation law at the interface boundary between refined domains requires only to balance the outward normal component of the flux vector. The solution is permitted to be discontinuous at the domain interface to satisfy the conservative property, and the approximate Riemann approach is well-posed [20,21]. However in solving the diffusion dominant partial differential equations for combustion, the function continuity and adjoint consistency of solutions between refined domains must be maintained across the interface and this issue has been known at the very beginning of the development of the polynomial refinement algorithms [15]. A wide range of procedures have been investigated from the penalty method [22] to the more recent studies on the recovery polynomial basis approaches [18,19,23,24]. The essential idea is rest on an effective coupling of the discontinuous solutions across the interface between locally refined domains which permits a very large class of solving schemes to be utilized [18,19]. This issue has been one of the focused areas of the present intensive basic research.

The inherent deficiency of the local polynomial refinement using Gauss Quadrature formulation at the interface of locally refined domains is remedied by a differential reconstruction scheme [18,19]. The continuous solution at the interface for combustion simulation is enforced by this approach for the diffusion dominant equation. A multiple-point, unequal spaced, differencing reconstruction approximation in preserving the spectral-like accurate and to increase computationally efficient has been accomplished. It is found that the shared first and second derivatives at the interface can be computed from the roots of polynomials of adjacent domains and effectively retains the numerical resolution in comparison with the recovery-based, L_2 norm projection, penalty, and reconstruction methods in applications [18,19,24]. The computed flame thickness agrees well with results using a systematic mesh refinement approach and experimental observation [8-10,18,19].

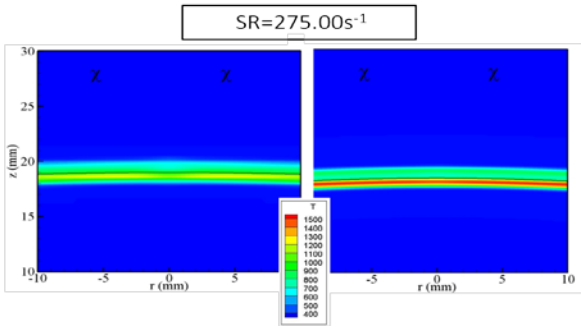

Figure 2. Detailed structure of stretched counter-flowing air-hydrogen flame

The intrinsic behavior of the present algorithm in practical applications has been successfully demonstrated for the counter-flowing, air-hydrogen combustion as shown in Figure 2. The highly stretched flame that approaching the extinct state is successfully simulated; the thin flame structure is accurately captured by the developed spectral method through the diminishing residual formulation [1]. Meanwhile, improvement has also been made to increase the convergence rate by addressed the flux vector balancing and continuity preserving condition across the interfaces of the immediately adjacent computational domains [10,18,19].

In order to cover a very wide range of computational simulations from the diffusive counter-flowing hydrogen flame to the ethylene/JP7 scramjet combustion, a system of robust and accurate numerical procedures becomes a critical element for modeling and simulation. The overall resolution also becomes an open issue when Riemann problem is invoked for shock capturing. The incurred Gibbs phenomenon in numerical solutions must be controlled by either adding artificial dissipation or using a post-process with low-pass filters [25]. The resultant numerical resolution is thereby uncertain. This concerned is also existed when applying a high order WENO scheme to solve hyperbolic conservation laws for flowfield with shock jumps, the improved numerical behavior is not derived from its superior accuracy at the critical points of the solution, but it rather gains through the larger weights assigning to stencils with discontinuities [26]. To address this concern, a comparative study of the adaptive polynomial local refinement and the compact-differencing up to sixth-order accuracy has been performed to assess the ability in defining the fine-structure of a diffusive flame and in sustaining supersonic combustion. For the compact-differencing scheme, the staged one-order-lower approximation for the transition operator between the interior domain and the far-field boundaries is used and this formulation is based on the summation-by-parts energy mode analysis [18,21,27].

The comparative investigation of the local grid refinement and the compact-differencing schemes are implemented by the diminishing residual algorithm [1,10,18,19]. In this procedure, the discretized partial differential system is first cast in the delta form in time, and then the equations are further split into different left-hand-side (LHS) and right-hand-side (RHS) differencing operator. The complete governing equation at any instance is retained on the RHS of the equation and is calculated by the high resolution numerical schemes. The LHS is required only to maintain computational stability to drive the iterative process to a vanishing temporal residual. Whence the residual has reached a designated criterion, the solution will yield the desired spectral-like accuracy correspond to the implemented local polynomial refinement or compact-difference schemes. A systematic evaluation of the high-resolution schemes in the high local gradient domain and its transient characteristic to the far field has been successfully accomplished [18,19,28].

The quantification of comparisons is first given by the temperature distribution along the center line of the heat source from combustion in Figure 3. The levels of the resolved temperature are affected by the discontinuous heat source distribution; the temperature by the windward scheme show numerical oscillation at the jumps and results in a much lower temperature, 980.73 K, and the numerical oscillations exhibit a magnitude of ±27.50 K at both terminal locations. There also is a difference between the predictions by the polynomial local refinement and the fourth-order compact-difference schemes. The former yields a value of 1120.00 versus the latter of 1100.00 K. At the edge of discontinuous heat source from combustion, the jumps are captured by the polynomial local refinement method in six unequal-spacing root points. The resolution by the compact-difference scheme requires two more equal-space points.

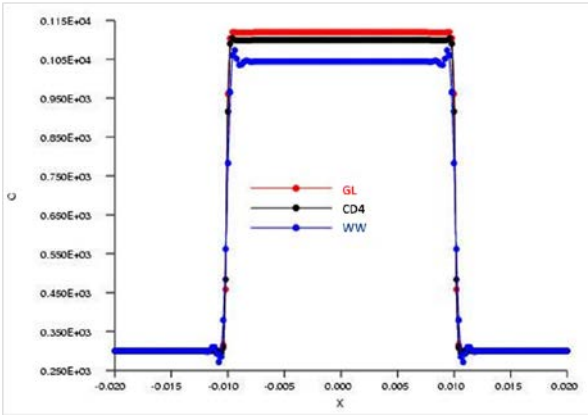

Figure 3. Comparison of nuemrical resolution at the heat source of combustion

The comparisons of the first and the second spatial derivatives along the centerline of the heat source from combustion are also obtained and depicted in Figures 4 and 5. In spite of the difference in the supporting mesh-point number density, the first and second derivatives by the polynomial local refinement and the compact-difference schemes in the middle of the global grid blocks are nearly identical to each other, to yield the absolute values of 0.2780×10^{6} versus 0.2746×10^{6} and 0.3292×10^{9} versus 0.3135×10^{9} respectively. The conventional windward approximation underpredicts the derivation by 23.6% with respect to the high-resolution procedures also shows numerical oscillations approaching and leaving the abruptly changing heat source locations. In short, both the high-resolution schemes exhibit a desired improvement over the windward approximation for determining the maximum attainable temperature along the heat source from combustion and

suppressing the oscillatory numerical behavior. These improvements in numerical resolution are essential for investigating the detailed flame structure with fine–scale vortical interactions.

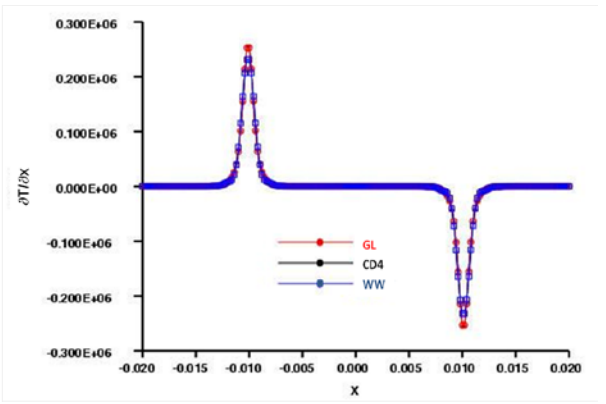

Fig. 4 Comparison of calculated first derivative ($\partial T/\partial x$) for the two-dimensional model equation

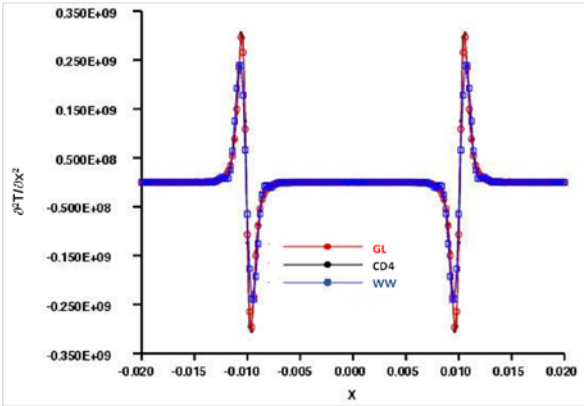

Fig. 5 Comparison of calculated second derivative ($\partial^2 T/\partial x^2$) for the two-dimensional model equation

Figure 6 presents the final assessment for the developed local polynomial refinement procedure based on the Gauss-Lobatto formulation by comparing the hydroxide concentration in molar fraction with the benchmark results of AFRL/RZ. This validating base is generated by the UNICORN program on the finest mesh available and the local polynomials refinement is achieved by16 global grid blocks with three different degrees of polynomial of 11, 25, and 51. The highest degree polynomial (51) is applied only in the 8th grid block ($17.5 \leq r \leq 20$ mm). The immediately adjacent grid blocks to the highest gradient domain are assigned the 25-degree polynomials and the 11-degree polynomials farther away from the high gradient region. The flame thickness determined from the radical component, OH, of the hydrogen-air combustion is slightly thinner than that of the molecular component of hydrogen. In essence, the flame thickness varies from chemical species to species according to the associated diffusion velocity and reaction rate. In essence, the flame thickness is best characterized by the thermal thickness of the flame. From the computational simulation, the counter-flow jet velocity exhibits a complex pattern which decelerates toward the flame and accelerates at the outer edge of the flame then finally reaches a free-stream stagnation point within the fame of the counter-flow combustion process. The complex flame structure is clearly governed by the molecular diffusion and the rate of species generation and recombination. An in-depth analysis can be achieved only by examining all chemical species within the flame.

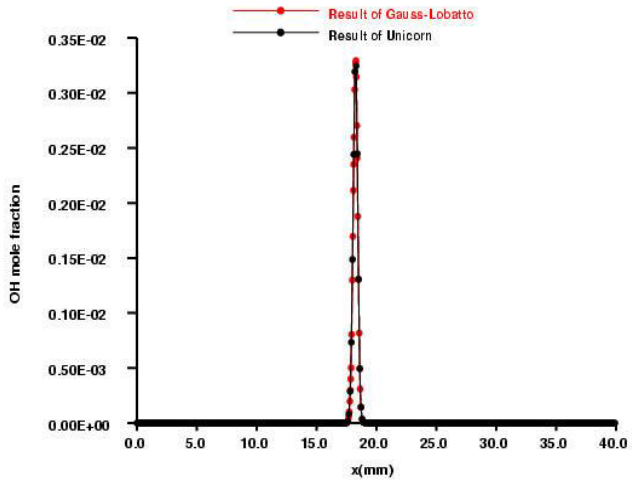

Fig. 6 Validated flame thickness by comparing with benchmark of AFRL/RZ (UNICORN)

The agreement between solutions of the present computational simulations with AFRL benchmark is excellent. The maximum discrepancy between the two results is 4.172×10^{-3} in molar fraction of hydroxide, and is less than 0.23×10^{-2} mm in predicted flame thickness of 2.07 mm. However, the finest grid spacing for the locally refined computational domain is 7.194×10^{-5} mm and the detailed flame structure is described by 29 polynomial roots. It is important to note that the solution using Gauss-Lobatto formula can still be refined through the adaptation of an even higher and unlimited degree of polynomial. For the present simulation condition, a total of 243 root points of the Legendre polynomial are used. The validating agreement between results is anticipated because of the shared kinematic and thermodynamic data from the UNICORN program. The most important and meaningful conclusion can be drawn from this comparison is that the Gauss-Lobatto formulation has the desired resolution characteristic for the intermediate wave number within a flame. It offers a potentially great advantage in practical application for combustion simulation.

The basic research for the development of a high performance and high resolution local polynomial refinement method in a steep gradient domain has been successfully developed and validated for combustion simulation. In a comparative investigation with a sixth-order compact differencing procedure, the finest local grid spacing for resolving the flame by the local polynomial refinement has reached a value less 7.194×10^{-5} mm which is previously unattainable. The verified numerical method has successfully applied to a counter-flowing, stretched hydrogen-air jet flame. The research results substantiate the finding for the criterion of a minimum flame thickness for determining the applicability of the flamelet concept – a vortex with a dimension even less than one millimeter will distort a thin flame structure for countering-flow hydrogen combustion [3,8,9].

In an effort to accelerating the technical transition to Air Force Research Laboratory, a preliminary investigation has been carried out for combustion within a hypersonic hydrogen-air scramjet. This activity is designed primarily as a path-finding effort to quantify the radiative heat transfer within the combustion chamber of a scramjet with nonequilibrium chemical reactions. Additional information is also sought in the scaling of combustor in regarding to the ignition delay. The overall length of the simulated scramjet is 140 cm with a cylindrical combustor with the dimensions of 100×17.7 cm. The entire computational domain of the axisymmetric configuration is resolved by 43,710 cells. The inlet Mach number is assigned a value of 5.21 and the fuel is injecting into the combustor at a speed of 600 m/s and at a pressure of 2 Atm. The chemical kinetic model of the hydrogen-air combustion consists of a system of eight elementary chemical reactions for an un-premixed supersonic hydrogen flame [11]. For the inlet shock capturing, the Riemann solver is implemented. The developed local polynomial refinement therefore is applying only for the nonequlibrium chemical reacting flow within the combustor to achieve a high numerical resolution.

Figure 7 shows the essential features of the nonequilibrium chemical reactions downstream of the isolator with multiple fuel ejectors. The temperature profiles of the nonequilibrium chemical reactions before and after the flame ignited is presented together to highlight the combustion delay and energy release pattern. The numerical solutions can only be validated by comparing with theoretic analyses and known data in the open literature [28,29]. All computational results, including an initiating global chemical kinetic model reveal the ignition delay on the order of 1.32×10^{-2} seconds. The present computational result indicates that the chemical kinetic model indeed can adequately describe the chemical kinetic process and provides invaluable information for a design scaling of scramjet configurations. Furthermore, the complex flame structure within the combustion chamber is captured by the numerical simulation including the hot spot of the radiative energy exchange. Radiating heat transfer of the interdisciplinary numerical simulation is described by both the diffusion and flat-layer approximations and is found to be sufficient to model the additional energy exchange mechanism within the combustor, as well as, to the interior surface of the combustor. This interdisciplinary simulation has revealed the long overlooked heat protection consideration for the increasingly higher pressure and temperature propulsive systems. For this unique accomplishment, the developed interdisciplinary modeling and simulation capability is being transferred to Propulsion and Power Directorate of AFRL for hypersonic scramjet investigation by a task order for graduate students support.

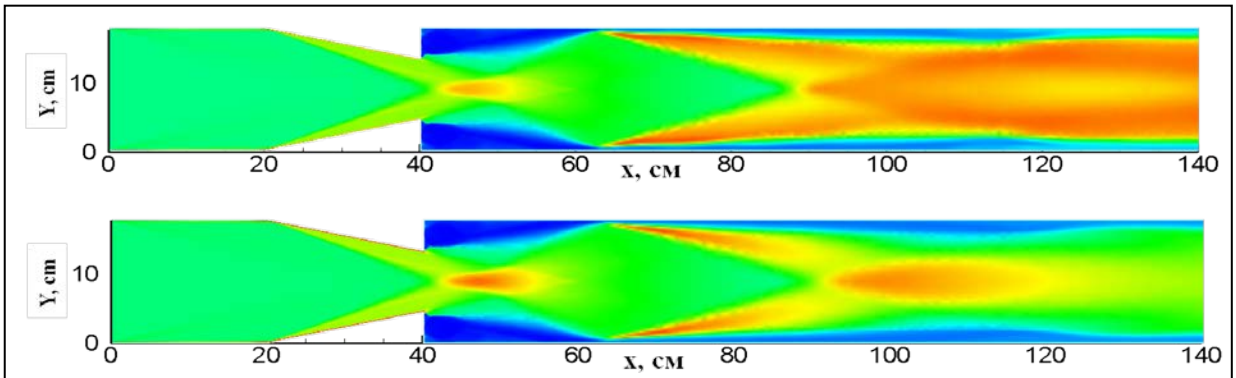

Fig. 7 Flow field structures in temperature contours within combustion chamber of scramjet

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Honors & Awards Received

USAF Basic Research Award, 1986
Fellow of AIAA, 1993
Outstanding and Exception Civilian Service Awards, 2001
AIAA Plasmadynamics and Laser Award, 2004

AFRL Point of Contact

Dr. Donald B. Paul, AFRL/RB WPAFB, OH 937-255-7329, met weekly until June 2011.
Dr. Richard Rivir, AFRL/RZ WPAFB, OH 937-255-2744. Sponsor for the FA8650-08-D-2806, Task Order 4, A path-finding study for radiative exchange in combustion chamber, interacted monthly.
Mr. Charles Brinks, USAF X51A Program Manager, AFRL/RZAT, WPAFB, 937-255-7611
Dr. Roger Kimmel, AFRL/RBAA WPAFB, OH 937-255-8295, interacted weekly.
Mr. Michael Zeigler, AFRL/RBAI WPAFB, OH 937-656-6307, interacted and met weekly.
Dr. Melvyn Roquemore, AFRL/RZ WPAFB, OH 937-255-6813
Dr. Biswa Ganguly, AFRL/RZ WPAFB, OH 937-255-6782

Transitions

The present basic research was initiated to introduce innovative numerical algorithms and to develop high-resolution, interdisciplinary simulation capability for combustion. Based on this long-term objective, the technical transitions are focused on the dissimilation of research results first to the research scientists of AFRL and then to national/international conferences of professional societies. All the technical transition processes are consistently followed up through personal interactions.

The most effective technical assist/transition activities can be summarized as (1) on September 2011, Maj. Gen. W.N. McCasland, Commander of Air Force Research Laboratory, invited the principal investigator to serve on the External Independent Review Team (EIRT) for performance views of the USAF X51A Scramjet system. (2) The AFOSR sponsored local grid refinement computational simulation for nonequilibrium combustion is expanded its applicability from combustion to include radiative heat transfer for advanced propulsion systems. The basic research team received a task order (FA8650-08-D-2806, Task Order 0004) for graduate student support from the Propulsion Directorate of the Air Force Research Laboratory to create a path-finding procedure to study the radiative exchange within combustor.

The additional technology assist effort to USAF includes the transition of the concept and potential practical applications of the Gaussian Quadrature to premixed- and non-premixed turbulent hydrogen combustion. A scientific interaction has been maintained with Dr. W. Melvyn Roquemore (AFRL/RZ 937-255-6813). The continuous exchange and collaboration has also been sustained with the combustion research group of the Propulsion Directorate. This activity has proved to be extremely mutual benefit in advancing basic understanding of extremely complex combustion phenomena for USAF's interest.

The new model and computational simulation for combustion have also been conveyed to Dr. Biswa Ganguly; a mutual support agreement for plasma assisted ignition and enhanced combustion stability has been reached in January 2010. The present project will provide a direct technical support to Center of Advanced Power and Energy Conversion of the joint Wright State University and Air Force Research Laboratory (AFRL/RZPE 937-255-6782).

New Discoveries

None.